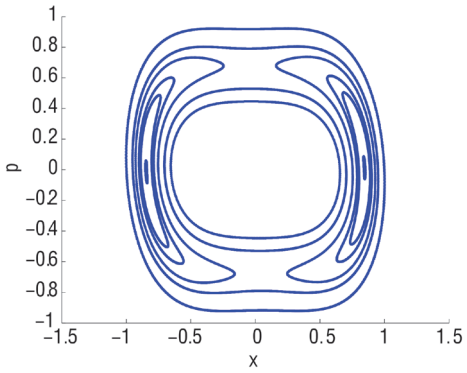
# Parametric Instabilities in Symplectic Integration with a Variable Time Step

**Andrew S. Richardson, John M. Finn, T-5**

There are good reasons to use variable time steps in ODE integrators, for example symplectic integrators for Hamiltonian systems. However, variable time steps based on an error estimator can introduce parametric resonances and, therefore, numerical instabilities. In this note we describe this process in the simplest terms, and indicate how these parametric instabilities can be avoided.

There are two commonly used approaches for numerical integration of Hamiltonian equations of motion. The first uses a symplectic integrator (a variational integrator[1]), which preserves the phase space structure of the system and can, for many purposes, be fairly low order in the time step. (Symplectic integrators are a special case of mimetic differencing.) The second approach is to use a high order but non-symplectic integrator, typically with an adaptive time step to obtain the highest accuracy. It is then argued that the loss of phase space structure is small due to the high accuracy of the scheme. If the time interval over which the integration is done is limited, this approach may be justified. For particle-in-cell (PIC) codes, low-order symplectic integrators are very commonly used, and those used are typically second-order accurate. When possible (when the Hamiltonian is separable, for example in electrostatic problems), leapfrog or Verlet integration is used. (In the presence of magnetic fields, a modification leads to the Boris algorithm.) In more general, non-separable, cases [1,2], modified leapfrog (ML) has been used effectively.

*Fig. 1. First-order Leapfrog, h(t) = h0 (1+ε sin(ω t)), h0=0.1, ε=0.5, ω=2*




There has been work in recent years related to using adaptive-time-step-symplectic integrators, with disappointing results. The difficulties have arisen in the form of numerical instabilities. We have recently identified the major problem as the occurrence of an instability associated with parametric resonance.

*[1]The distinction relates to the method of derivation. For the former, one goes from the Lagrangian to the Hamiltonian in the continuum and then discretizes, making sure that the phase space structure is preserved. For the latter, one discretizes the Lagrangian and does the variation on the discretized action. The resulting equations automatically preserve phase structure.*

To illustrate, we begin with the harmonic oscillator, with Hamiltonian $H = p^2/2m + m\omega_0^2 q^2/2$. With $P = p/\sqrt{m\omega_0}$, $Q = \sqrt{m\omega_0}q$, we have $H = \omega_0(P^2 + Q^2)/2$. First order leapfrog for this separable system gives:

$$Q(t_{n+1}) = Q(t_n) + h_n\omega_0 P(t_n) \qquad P(t_{n+1}) = P(t_n) - h_n\omega_0 Q(t_{n+1}),$$

where for this illustration the time step $h_n = h(t_n)$ depends on time explicitly. In the actual case discussed below, the time step $h(Q, P)$ is determined by an error estimate and depends on time implicitly through $Q(t), P(t)$. By the method of modified equation analysis, we find that this discrete system is approximated by:

$$\dot{Q} = \omega_0\left(\frac{\omega_0 h(t)}{2} - \frac{\omega_0^2 h\dot{h}(t)}{4}\right)Q + \omega_0\left(1 + \frac{\omega_0^2 h^2}{6}\right)P,$$

$$\dot{P} = -\omega_0\left(1 + \frac{\omega_0^2 h^2}{6}\right)Q - \omega_0\left(\frac{\omega_0 h(t)}{2} - \frac{\omega_0^2 h\dot{h}(t)}{4}\right)P,$$

or

$$H = \omega_0\left(1 + \omega_0^2 h^2/6\right)\left(P^2 + Q^2\right)/2 + \left(\omega_0 h(t)/2 - \omega_0^2 h\dot{h}(t)/4\right)QP.$$

If we take $h(t)$ to vary sinusoidally, $\sim h0(1 + \varepsilon\cos\omega_1 t)$, the term $\omega_0 h(t)QP/2$ in the Hamiltonian shows the presence of a first-order parametric resonance, giving instability for $|\omega_1/\omega_0 - 2| < \alpha\varepsilon$. Numerical investigations indeed show instability in this range. (The factor $1 + \omega_0^2 h^2/6$) multiplying the overall factor $P^2 + Q^2$ does not lead to a second-order parametric instability.)

Figure 1 shows the phase space for the quartic oscillator $H = p^2/2m +$

For more information contact John M. Finn at finn@lanl.gov.

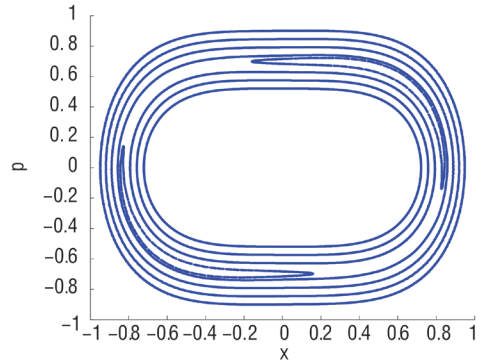
$q^2/2 + q^4/2$ obtained with first-order leapfrog integration using $h(t) = h_0(1 + \varepsilon\cos\omega_1 t)$. A set of nonlinear resonances or islands is visible on the surface where the nonlinear oscillator frequency is equal to $\omega_1/2$, a localized parametric resonance. The width of these islands' scales is $\varepsilon^{1/2}$, as expected. For comparison, the analogous plot using Crank-Nicolson (CN) integration (known to be symplectic but also time-centered) shown in Fig. 2 has much thinner islands, and a modified equation analysis of CN shows only higher-order parametric resonances. Staggered, or symmetrized, leapfrog also has only second-order parametric instabilities, and has numerical results similar to those shown in Fig. 2 for CN. However, recent work has shown that leapfrog (and ML for non-separable systems) has one great advantage over CN or other methods in a PIC code—it allows *all* the particle positions to be updated before the code solves for the field [2]. For CN and many other schemes, the fields need to be found after *each* particle is moved, a terrible disadvantage. Thus, it appears that the best strategy involves using leapfrog, or ML if necessary, to second-order accuracy.

In real problems, the time step is not given explicitly as a function of time, but rather computed from an error estimate, which depends on the position in phase space. (Leapfrog requires modification to remain a symplectic integrator with $h = h(Q, P)$, but that is easily done.) For example, for the Harmonic oscillator above the error estimate leads to a time step depending quadratically on $Q, P$, leading to a $\cos 2\phi$ dependence of the time step $h$. (The quantities $(\phi, J = (P^2 + Q^2)/2)$ are action-angle variables.) This therefore leads in first-order leapfrog to a first-order parametric resonance exactly like the $\omega_1/\omega_0 = 2$ resonance above.

For applications such as PIC in which CN cannot be used, but a symplectic integrator is needed, the best strategy is this—use a higher-order symplectic integrator such as symmetrized ML and limit the time step size, and perhaps the variation of the time step, to minimize the effects of parametric resonance.

One other point that should be made is that the parametric instabilities described above apply also to non-symplectic integrators. However, the instabilities may not be recognizable as such because non-symplectic integrators can introduce damping, and the parametric instability would need to overcome this damping to be observable.

*Fig. 2. Crank–Nicolson, h(t) = h0 (1+ε sin(ω t)), h0=0.1, ε=0.5, ω=2.*




[1] Finn, J.M. and L. Chacon, *Phys Plasma* **12**, 054503 (2005).
[2] Fichtl, C.A., "An Arbitrary Curvilinear Coordinate Particle In Cell Method," PhD dissertation, 2010.

**Funding Acknowledgments**
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